

## View of End Points for a Data Set

Sponsor	<input type="text" value="1100021"/>	<input type="text" value="Albemarle Corporation"/>	Create Date:	<input type="text" value="12/16/03"/>
CAS No	<input type="text" value="77098078"/>	<input type="text" value="1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene"/>		
Consortia	<input type="text"/>	<input type="text"/>		

### Physical/Chemical Properties

- ☐
- ☐
- ☐
- ☐
- ☐

### Environmental Fate

- ☐
- ☐
- ☐
- ☐

### Ecotoxicity

- ☐
- ☐
- ☐

### Health

- ☐
- ☐
- ☐
- ☐
- ☐
- ☐

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# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Water Solubility

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

Revision Date:

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimation

>> GLP No

>> Year study performed 2003

## Remarks for Method

The water solubility was estimated by the WSKOW model of EPIwin (v3.04). Only the molecular structure was entered into the program.

## Results

>> Precision

=

>> Water Solubility Value

0

>> Upper Value

0

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Water Solubility

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

>> Unit mg/L

>> Temperature 25

>> Solubility Category Insoluble

>> pH Value 55

>> pKa Value 55

## Results Remark

pH and pKa are not applicable. The water solubility was estimated using a computer program.

## Conclusions

The estimated water solubility is 0.05697 mg/L.

## Data Quality

Reliability

## Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Water Solubility

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

## Reference

### >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5-tetrabromo-, mixed esters with diethylene glycol and propylene glycol

## Chemical Category

## Method

>> Method/Guideline followed

Other

>> GLP

No

>> Year study performed

1978

>> Species

rat

>> Strain

Sprague-Dawley

>> Sex

Both

>> Number of males per dose

5

>> Number of females per dose

5

>> Vehicle

corn oil

>> Route of Administration

Oral

Remarks for Method

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Boiling Point

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

1/8/04

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> GLP No

>> Year study performed 2003

## Results

### Remarks for Method

The boiling point was estimated using the MPBPWIN module of EPIwin. Only the molecule structure was entered into the program.

>> Precision

=

>> Boiling Point Value

538

>> Upper Value

0

>> Unit °C

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Boiling Point

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

>> Pressure

760

>> Pressure Unit

mm Hg

>> Decomposition

No

Results Remark

## Conclusions

The boiling point was estimated to be 537.52 degrees C.

## Data Quality

Reliability

Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Boiling Point

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## Reference

### >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General



# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Melting Point

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

1/8/04

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> GLP No

>> Year study performed 2003

## Remarks for Method

The melting point was estimated by the MPBPWIN module of EPIwin (v3.04). Only the molecular structure was entered into the program.

## Results

>> Precision =

>> Melting Point Value 230

>> Upper Value 0

>> Unit °C

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Melting Point

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

>> Decomposition

>> Sublimation

## Results Remark

## Conclusions

The estimated melting point is 230.13 degrees C.

## Data Quality

Reliability

## Data Reliability Remarks

## Reference

### >> Remarks

All estimations on this substance were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Melting Point

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## General

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Partition Coefficient

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:  
12/16/03

## Test Substance

Remarks 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> GLP No

>> Year study performed 2003

## Remarks for Method

The partition coefficient was estimated by the KOWWIN module of EPIwin (v3.04). Only the molecular structure was entered into the program.

## Results

>> Precision

=

>> Value of Log Pow

3.82

>> Upper Value

0

>> Temperature

25

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Partition Coefficient

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## Results Remark

## Conclusions

The log Kow was estimated to be 3.82.

## Data Quality

Reliability

## Data Reliability Remarks

## Reference

### >> Remarks

All estimations on this substance were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Partition Coefficient

Sponsor ID 1100021

Albemarle Corporation

Create Date 12/16/03

CAS Number 77098078

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed  
esters with diethylene glycol and propylene glycol

Study Number 1

Consortia ID

Completed: Y

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Vapor Pressure

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> GLP No

>> Year study performed

2003

## Remarks for Method

The vapor pressure was estimated by the MPBPWIN module of EPIwin (v3.04). Only the molecular structure was entered into the program.

## Results

>> Precision

=

>> Vapor Pressure Value

2.37E-14

>> Upper Value

0

# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Vapor Pressure

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

>> Unit mm Hg

>> Temperature 25

>> Decomposition No

## Results Remark

## Conclusions

The vapor pressure was estimated to be  $2.37 \times 10^{-14}$  mm Hg using the Modified Grain Method.

## Data Quality

Reliability

## Data Reliability Remarks

## Reference



# EPA High Production Volume (HPV) Track

Physical-Chemical End Point:  
Vapor Pressure

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Stability in Water

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

1/8/04

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> Test Type

Abiotic

>> GLP

No

>> Year study performed

2003

Remarks for Method

The aqueous hydrolysis rate constants were estimated by the HYDROWIN module of EPIwin. Only the molecular structure was entered into the program.

## Results

>> Nominal concentration

Not applicable

>> Measured concentration

Not applicable

>> Precision

=

>> Hydrolysis Result

1

>> Upper Value

0

>> Unit

Days

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Stability in Water

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

>> pHVal 8

>> Temperature 25 degrees C

>>Breakdown products Unknown

## Results Remarks

The program selected the chemical class 'esters' for the estimation. HYDROWIN calculates a base-catalyzed rate constant for esters. For most esters, the base-catalyzed rate constant is dominant.

## Conclusions

The estimated hydrolysis rate constant ( $K_b$ ) for  $\text{pH} > 8$  is 5.886 L/mol-sec. The estimated half-life at  $\text{pH} 8$  is 1.363 days. The estimated half-life at  $\text{pH} 7$  is 13.629 days.

## Data Quality

Reliability

## Data Reliability Remarks

Fragments(s) on this compound were not available from the fragment library and substitute(s) were used. Also, ortho-position fragment(s) on phenyl ring were not considered by the model.

## Reference

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Stability in Water

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Biodegradation

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

Revision Date:

2/2/04

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> Test Type

aerobic

>> GLP No

>> Year study performed 2003

>> Contact Time 0

>> Inoculum

None

## Remarks for Method

The potential for the substance to biodegrade was estimated using the BLOWIN module of EPIWin. Only the chemical structure was entered.

## Results

>> Precision range

>> Degradation Value 0

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Biodegradation

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

>> Upper value 0

>> Time Frame 0

>> Time Units

>> Breakdown products Unknown

Results Remarks

## Conclusions

The program estimated that the substance would not biodegrade fast using either a linear or non-linear model prediction. The program also estimated that the ultimate biodegradation timeframe was months and the primary biodegradation timeframe, weeks.

The module defines these terms as the following. The numerical definition of "biodegrades fast" or "does not biodegrade fast" was not provided in the module. Ultimate biodegradation is the transformation of a parent compound to CO<sub>2</sub> and H<sub>2</sub>O. Primary biodegradation is the transformation of a parent compound to an initial metabolite.

## Data Quality

Reliability

Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Biodegradation

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

## Reference

### >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Photodegradation

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

Revision Date:

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

### >> Method/Guideline followed

Estimated

### >> Light Source

Not applicable

### >> Light Source Spectrum in nm

0

### >> Relative Intensity

Not applicable

### >> Absorption Spectrum of Substance

Not applicable

### >> GLP

No

### >> Year study performed

2003

### Remarks for Method

The rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and the molecule was estimated using the AOPWIN module of EPIwin. The estimated rate constant is used by the program to calculate the atmospheric half-life of the molecule based upon average atmospheric concentrations of hydroxyl radicals and ozone.

Only the molecular structure was entered into the program.

## Results

### >> Concentration Value

0

### >> Unit

Days

### >> Temperature

Not specified



# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Photodegradation

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

>> Direct Photolysis Precision =

>> Direct Photolysis 0

>> Direct Photolysis Upper value 0

>> Direct Photolysis Unit Days

>> Indirect Photolysis Precision

>> Indirect Photolysis 0

>> Indirect Photolysis Upper value 0

>> Indirect Photolysis Unit

>> Sensitizer xxx

>> Sensitizer Concentration

>> Sensitizer Unit

>> Rate Constant xxx

>> Breakdown products Unknown

Results Remark

Conclusions

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point:  
Photodegradation

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

The overall OH rate constant was estimated to be  $30.51 \times 10^{(-12)}$  cm<sup>3</sup>/molecule-sec. The half-life was estimated to be 0.351 days based on a 12-hr day and  $1.5 \times 10^{(6)}$  OH/cm<sup>3</sup>.

## Data Quality

Reliability

## Data Reliability Remarks

## Reference

## >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point: Transport between Environmental Compartments (Fugacity)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> Test Type

Level III fugacity model

>> Year study performed

2003

## Remarks for Method

The transport between environmental compartments and environmental partitioning was estimated using a Level III Fugacity Model, EPIwin. Only the molecule structure was entered into the program.

Emissions to air, water, soil and sediment set at 1000, 1000, 1000 and 0 kg/hr, respectively

## Results

>> Media

Air 0.0008%, Water 15.6%; Soil 82.3%; Sediment 2.04%

>> Distribution Concentration

Fugacity (atm): Air  $4.39 \times 10^{-20}$ , Water  $1.6 \times 10^{-21}$ , Soil  $1.4 \times 10^{-21}$ , Sediment  $1.6 \times 10^{-21}$

Reaction (kg/hr): Air 3.27, Water 358, Soil  $1.9 \times 10^3$ , Sediment 12

Advection (kg/hr): Air 0.4, Water 743, Soil 0, Sediment 2

Reaction (%): Air 0.1, Water 12, Soil 63, Sediment 0.4

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point: Transport between Environmental Compartments (Fugacity)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Advection (%): Air 0.01, Water 25, Soil 0, Sediment 0.06

## Results Remark

Henry's LC:  $2.74 \times 10^{-16}$  atm-m<sup>3</sup>/mole  
Vapor Presss:  $2.37 \times 10^{-14}$  mm Hg  
Liquid VP:  $2.53 \times 10^{-12}$  mm Hg (super-cooled)  
Melting Pt: 230 deg C  
Log Kow: 3.83  
Soil Koc:  $2.77 \times 10^{+3}$

## Conclusions

If released to the environment, the molecule is expected to partion to soil (82%). Predicted partitioning to water (15%) and sediment (2%) are much less. Negligible partitioning is anticipated to air (0.0008%).

## Data Quality

Reliability

## Data Reliability Remarks

## Reference

## >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Environmental Fate and Pathway End Point: Transport  
between Environmental Compartments (Fugacity)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Fish

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol

## Chemical Category

## Method

### >> Method/Guideline followed

Conducted prior to established guidelines.

### >> Test Type

static

### >> GLP

No

### >> Year study performed

1979

### >> Species

Lepomis macrochirus

### >> Analytical monitoring

No data

### >> Exposure period

96 hours

### >> Statistical Method

Not known

## Remarks for Method

Bluegill sunfish were exposed to concentrations of 10, 18, 32, 56 and 100 mg/L. Acetone was the vehicle. All test concentrations were cloudy with the top 2 doses completely opaque.

## Results

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Fish

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

>> Nominal concentration 10, 18, 32, 56, 100

>> Measured concentration No data

>> Precision =

>> Endpoint Type LC50

>> Endpoint Value 12 >> Unit used mg/L

>> Concentration Type Nominal >> Endpoint Time 96

## >> Statistical results

The 95% confidence interval limits were 1-18 mg/L.

## Results Remark

## Conclusions

The 96 hr LC50 in bluegill sunfish was 12 mg/L.

## Data Quality

Reliability

## Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Fish

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## Reference

### >> Remarks

Thompson, C, Forbis A. 1979. Acute toxicity of FM PHT-4 Diol (EX-1) to Bluegil sunfish (*Lepomis macrochirus*). Analytical Bio Chemistry Laboratories, Inc.

## General



# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Fish

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	Y

Revision Date

2/2/04

## Test Substance

Remarks

1,2-benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

### >> Method/Guideline followed

Estimated

### >> Test Type

static

>> GLP No

>> Year study performed 2003

### >> Species

Not applicable

>> Analytical monitoring Not applicable

>> Exposure period 96 Hours

>> Statistical Method Not applicable

### Remarks for Method

The ECOSAR module of EPIWIN was used to estimate the EC50 in fish for this substance. Only the chemical structure was entered into the software program.

The ECOSAR calculated the water solubility to be 37.96 mg/L. This is very different from the water solubility calculated by WSKOW, another module in EPIWIN, 0.5697 mg/L at 25 deg C.

## Results

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Fish

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	Y

>> Nominal concentration Not applicable

>> Measured concentration Not applicable

>> Precision =

>> Endpoint Type LC50

>> Endpoint Value 10 >> Unit used mg/L

>> Concentration Type Nominal >> Endpoint Time 96

>> Statistical results  
Not applicable

Results Remark

## Conclusions

The 96 Hour LC50 was estimated to be 9.973 mg/L.

## Data Quality

Reliability

Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Fish

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	Y

## Reference

### >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Aquatic Invertebrates

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

## Test Substance

2/2/04

Remarks

1,2-benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

>> Method/Guideline followed

Estimated

>> Test Type

static

>> GLP No

>> Year study performed 2003

>> Species

Daphnia sp.

>> Analytical monitoring Not applicable

>> Exposure period 48 Hours

>> Statistical Method Not applicable

## Remarks for Method

The ECOSAR module of EPIWIN was used to estimate the EC50 in Daphnid for this substance. Only the chemical structure was entered into the software program.

The ECOSAR calculated the water solubility to be 37.96 mg/L. This is very different from the water solubility calculated by WSKOW, another module in EPIWIN, 0.5697 mg/L at 25 deg C.

## Results

2/5/04

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Aquatic Invertebrates

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

>> Nominal concentration Not applicable

>> Measured concentration Not applicable

>> Precision =

>> Endpoint Type LC50

>> Endpoint Value 11

>> Unit used mg/L

>> Concentration Type Nominal

>> Endpoint Time 48

>> Statistical results

Not applicable

Results Remark

## Conclusions

The 48 Hour EC50 in Daphnids was estimated to be 10.779 mg/L.

## Data Quality

Reliability

Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point:  
Acute Toxicity to Aquatic Invertebrates

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## Reference

>> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point :  
Toxicity to Aquatic Plants

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

Revision Date:

2/2/04

## Test Substance

Remarks 1,2-benzenedicarboxylic acide, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester

## Chemical Category

## Method

### >> Method/Guideline followed

Estimated

### >> Test Type

static

### >> GLP

No

### >> Year study performed

2003

### >> Species

Green algae

### >> End Point

EC50

### >> Analytical monitoring

Not applicable

### >> Exposure period

96 Hour

### >> Statistical Method

Not applicable

## Remarks for Method

The ECOSAR module of EPIWIN was used to estimate the LC50 in green algae for this substance. Only the chemical structure was entered into the software program.

The ECOSAR calculated the water solubility to be 37.96 mg/L. This is very different from the water solubility calculated by WSKOW, another module in EPIWIN, 0.5697 mg/L at 25 deg C.

## Results

2/5/04

# EPA High Production Volume (HPV) Track

Ecotoxicity End Point :  
Toxicity to Aquatic Plants

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

>> Nominal concentration Not applicable

>> Measured concentration Not applicable

>> Precision =

>> Endpoint Type EC50-CD

>> Endpoint Value 1 >> Unit used mg/L

>> Concentration Type Nominal >> Endpoint Time 96

>> NOEC Precision >> NOEC 0 >> Unit used

>> NOEC Concentration Type

>> NOEC Effect(s) assesse

>> LOEC Precision >> LOEC 0 >> Unit used

>> LOEC Concentration Type

>> LOEC Effect(s) assesse

>> Response of Control Group (was it satisfactory?)

>> Statistical results

Results Remark

Conclusions



# EPA High Production Volume (HPV) Track

Ecotoxicity End Point :  
Toxicity to Aquatic Plants

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	N

The estimated 96 hour EC50 in green algae for this substance was 0.849 mg/L.

ECOSAR calculated the water solubility to be 37.96 mg/L. This is very different from the water solubility calculated by WSKOW, another module in EPIWIN, 0.5697 mg/L at 25 deg C.

## Data Quality

Reliability

## Data Reliability Remarks

## Reference

## >> Remarks

All estimations were performed using EPI WIN Suite, V.3.04, Syracuse Research Corporation, North Syracuse, New York.

## General

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

12/16/03

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5-tetrabromo-, mixed esters with diethylene glycol and propylene glycol

## Chemical Category

## Method

>> Method/Guideline followed

Other

>> GLP

No

>> Year study performed

1978

>> Species

rat

>> Strain

Sprague-Dawley

>> Sex

Both

>> Number of males per dose

5

>> Number of females per dose

5

>> Vehicle

corn oil

>> Route of Administration

Oral

Remarks for Method

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Observations were recorded during the first 4 hours post-dosing, at 24 hours and daily thereafter for 14 days.

## Results

>> Precision >

>>Acute Lethal Value 10000

>> Unit mg/kg-bw

>> Deaths per Dose

No deaths occurred.

## Results Remark

## Conclusions

The LC50 oral was > 10,000 mg/kg.

## Data Quality

Reliability

## Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## Reference

### >> Remarks

Dean W. Acute toxicity studies in rabbits and rats - PM PHT-4Diol. International Research and Development Corp. # 163-592. 29 June 1978.

## General

Sponsored by Velsicol.

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	N

Revision Date:

2/4/04

## Test Substance

Remarks 1,2-Benzenedicarboxylic acid, 3,4,5-tetrabromo-, mixed esters with diethylene glycol and propylene glycol

## Chemical Category

## Method

>> Method/Guideline followed

Other

>> GLP Unknown

>> Year study performed 1978

>> Species

rat

>> Strain Charles River CD

>> Sex Both

>> Number of males per dose

5

>> Number of females per dose

5

>> Vehicle Not applicable

>> Route of Administration

Inhalation

Remarks for Method

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	N

Five male and five female rats were exposed for one hour to a saturated vapor concentration of the test substance. The concentration of the vapor was calculated to be 0.008 mg/L.

## Results

>> Precision >

>>Acute Lethal Value 0

>> Unit mg/L(air)

>> Deaths per Dose

No deaths occurred during the exposure or the 14-day observation period.

## Results Remark

All rats were sacrificed at the end of the study and necropsied. No gross lesions were observed.

## Conclusions

The one hour LC50 was greater than the highest concentration tested, 0.008 mg/L. This represented a saturated concentration.

## Data Quality

Reliability

## Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	N

## Reference

### >> Remarks

Leong, B. Acute inhalation toxicity study in rats - FM PHT-4 DIOL. International Research and Development Corp. #163-599, 30 Aug 1978.

## General

Sponsored by Velsicol.

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	3
Consortia ID			Completed:	Y

Revision Date:

2/4/04

## Test Substance

Remarks 1,2-Benzenedicarboxylic acid, 3,4,5-tetrabromo-, mixed esters with diethylene glycol and propylene glycol

## Chemical Category

## Method

### >> Method/Guideline followed

Other

>> GLP Unknown

>> Year study performed 1978

### >> Species

rabbit

>> Strain New Zealand white

>> Sex Both

>> Number of males per dose 2 >> Number of females per dose 2

>> Vehicle None

### >> Route of Administration

Dermal

Remarks for Method



# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	3
Consortia ID			Completed:	Y

The test substance was applied to clipped sites on the backs of 2 male and female albino rabbits. Just prior to dosing the sites on one male and one female were abraded; those of the other two remained intact. The test material was applied at a dose of 20,000 mg/kg and the application sites were wrapped with gauze bandaging and overwrapped with Saran Wrap and several layers of Elastoplast tape. After 24 hours, the bandages were removed and the sites washed with water and examined. Examinations were repeated daily for 14 days.

## Results

>> Precision >

>> Acute Lethal Value 20000

>> Unit mg/kg-bw

>> Deaths per Dose

No animals died on test.

## Results Remark

No animals died, and all appeared normal during the 14-day observation period. Very slight to slight erythema, edema and atonia were noted during the observation period.

## Conclusions

The dermal LD50 was > 20,000 mg/kg, the highest dose tested.

## Data Quality

Reliability

## Data Reliability Remarks

# EPA High Production Volume (HPV) Track

Toxicity End Point:  
Acute Toxicity

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	3
Consortia ID			Completed:	Y

## Reference

### >> Remarks

Dean W. Acute toxicity studies in rabbits and rats - PM PHT-4Diol. International Research and Development Corp. # 163-592. 29 June 1978.

## General

Sponsored by Velsicol

# EPA High Production Volume (HPV) Track

Toxicity End point:  
Toxicity in Vitro (Gene Mutations)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

Revision Date:

2/4/04

## Test Substance

Remarks

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol.

## Chemical Category

## Method

### >> Method/Guideline followed

Other

### >> Test Type

Ames test

### >> System of Testing

Bacterial

### >> GLP

Unknown

### >> Year study performed

1977

### >> Species

Salmonella typhimurium, Saccharomyces (D4)

### >> Metabolic Activation

Tested with and without metabolic activation

### >> Concentration

0.001, 0.01, 0.1, 1.0 ug/plate

### >> Statistical Method

Not provided in IUCLID summary

### Remarks for Method

# EPA High Production Volume (HPV) Track

Toxicity End point:  
Toxicity in Vitro (Gene Mutations)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## Results

>> Result Negative

>> Cytotoxic Concentration

Not provided in IUCLID summary

>> Genotoxic Effects Unconfirmed

>> Statistical results

Not provided in IUCLID summary

Results Remark

## Conclusions

The test compound did not demonstrate mutagenic activity either with or without metabolic activation.

## Data Quality

Reliability

Data Reliability Remarks

## Reference

# EPA High Production Volume (HPV) Track

Toxicity End point:  
Toxicity in Vitro (Gene Mutations)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	1
Consortia ID			Completed:	Y

## >> Remarks

Brusick D. Mutagenicity evaluation of 859-82-4. Litton Bionetecs, LBI project #2683. March 1977.

## General

Sponsored by Velsicol Chemical Corp.

# EPA High Production Volume (HPV) Track

Toxicity End point:  
Toxicity in Vitro (Gene Mutations)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	Y

Revision Date:

2/4/04

## Test Substance

Remarks 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol.

## Chemical Category

## Method

### >> Method/Guideline followed

Other

### >> Test Type

Ames test

### >> System of Testing

Bacterial

### >> GLP

Yes

### >> Year study performed

1985

### >> Species

Salmonella typhimurium

### >> Metabolic Activation

Arochlor 1254-induced rat liver S-9 fraction

### >> Concentration

0, 50, 100, 500, 1000, 5000 ug/plate

### >> Statistical Method

Not available.

### Remarks for Method

Saytex RB 79 Diol was tested in Salmonella strains TA1535, TA1537, TA98 adn TA100 with and without metabolic activation. The test article was not soluble at the highest dose. Each dose was tested in triplicate. An untreated control, solvent control and positive control were tested concurrently.

# EPA High Production Volume (HPV) Track

Toxicity End point:  
Toxicity in Vitro (Gene Mutations)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	Y

## Results

>> Result Negative

>> Cytotoxic Concentration

Toxic in all strains at 5000 ug/plate.

>> Genotoxic Effects Unconfirmed

>> Statistical results

Not available.

### Results Remark

The test article did not casue a dose related increase in mutant colonies in any strain either with or without metabolic activation.

## Conclusions

The test article was not mutagenic.

## Data Quality

Reliability

### Data Reliability Remarks

## Reference

# EPA High Production Volume (HPV) Track

Toxicity End point:  
Toxicity in Vitro (Gene Mutations)

Sponsor ID	1100021	Albemarle Corporation	Create Date	12/16/03
CAS Number	77098078	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	Study Number	2
Consortia ID			Completed:	Y

## >> Remarks

Johnson and Mulholland. 1985. Genetic Toxicology Salmonella/Microsomal Assay. Ames 091-#089. Saytex RB79. Genetic Toxicology Laboratory. Ethyl Technical Center. Baton Rouge, LA.

## General

Sponsor: Ethyl Corporation, Baton Rouge, LA.